MOLECULAR DOCKING TECHNIQUE FOR SCREENING OF COMBINATORIAL LIBRARIES

Abstract of the Disclosure

A high-throughput molecular docking facility is presented for screening combinatorial libraries to identify binding ligands and ultimately pharmaceutical compounds. The facility employs a pre-docking conformational search to generate multiple solution conformations of a ligand. The molecular docking facility includes: generating a binding site image of the protein, the binding site image having multiple hot spots; matching hot spots of the binding site image to atoms in at least one solution conformation of the multiple solution conformations of the ligand to obtain at least one ligand position relative to the protein in a ligand-protein complex formation; and optimizing the at least one ligand position while allowing translation, orientation and rotatable bonds of the ligand to vary, and while holding the protein fixed.